Claims

1. A computer-implemented method comprising determining concave areas on an irregular computer model surface by intersecting the surface with a number of planar slices, determining, for at least two slices, parameters based on the intersection between the surface and the slice, and using the at least two determinations to determine a preferred concave region of the surface.

2. The method of claim 1, further including, for at least one slice, determining a closed volume bounded by only the surface and the slice.

3. The method of claim 1, further including, for at least one slice, determining a closed volume bounded by the surface, a slice, and one or more planes that are perpendicular to the slice.

4. The method of claim 1, further including, for at least one slice, determining a closed volume bounded by the surface, a slice, and a plane parallel to the slice.

5. The method of claim 1, further including, for a first slice, determining a closed volume bounded by only the surface and the first slice; for a second slice, determining a closed volume bounded by the surface, the second slice, and one or more planes that are perpendicular to the second slice; and for a third slice, determining a closed volume bounded by the surface, the third slice, and a plane parallel to the third slice.

6. The method of claim 1, wherein the surface is the calculated surface of a DNA molecule.

7. The method of claim 1, wherein the surface is the calculated surface of an RNA molecule.

8. The method of claim 1, wherein the concave areas on the surface are ranked according to the volume encompassed by the surface and the slice.

9. The method of claim 1, wherein the concave areas on a given surface are ranked according to the pocket opening area created by the intersections of the surface and the slice.

10. The method of claim 1, wherein the concave areas on a given surface are ranked according to a function of both the volume encompassed by the surface and the slice, and the pocket opening area created by the intersections of the surface and the slice.

11. The method of claim 1, wherein the surface is the calculated surface of a protein.

12. The method of claim 11, further including, for a first slice, determining a closed volume bounded by only the surface and the slice; for a second slice, determining a closed volume bounded by the surface, the slice, and one or more planes that are perpendicular to the slicing plane; and for a third slice, determining a closed volume bounded by the surface, the slice, and a plane parallel to the slice.

13. The method of claim 11, further comprising using a portion of the surface intersected by the slice and measuring binding affinity at the portion of the surface.

14. The method of claim 11, further comprising determining protein pockets including pockets bonded only by the surface and the slice pockets bonded by the surface and the slice, and a plane parallel to the slice, and pockets bonded by the surface, the slice, and one or more planes perpendicular to the slice.

15. The method of claim 14, further comprising ranking the pockets according to area of the slice bonded by the surface and any perpendicular planes and/or the volume enclosed by the surface, the slice, and the additional perpendicular or parallel planes.

16. The method of claim 14, further comprising determining, for at least some of the pockets which overlap, the aggregate volume and surface area thus made available for binding by small molecules.

17. The method of claim 14, further comprising, for at least some of the pockets, partitioning the pockets or an aggregate of at least some of the pockets into separate volumes and surface areas that can be occupied by a small molecule binding to the protein.

18. A computer-implemented method comprising:

intersecting a computer model of a protein surface with a series of slices; and

determining for a number of the slices concave areas of the protein surface that are more or less likely for a ligand molecule to bind to the protein.

19. The method of claim 18, further comprising using a specific determined concave area to determine binding affinity for a ligand.

20. The method of claim 19, wherein determining binding affinity includes quantizing the concave area and potential ligands and ranking complementarity there between.

21. A method comprising:

determining concave areas on a surface of a three dimensional computer model of a biomolecule by intersecting the surface with a number of planar slices;

determining, for at least two slices, parameters based on the intersection of the surface and the slices; and

using the determinations to determine a preferred ligand affinity region of the surface.

22. The method of claim 21, wherein the size and shape of the ligand affinity region are used to design a ligand tailored to that affinity region.

23. The method of claim 21, further comprising using a docking method to measure a potential binding affinity to a desired affinity region.

24. The method of claim 21, wherein a volume encompassed by the slice and the surface are determined for each slice.

25. The method of claim 21, wherein the area of intersection between the slice and the surface is determined for each slice.

26. The method of claim 21, further comprising quantizing the ligand affinity region and potential ligands into a cubic format, and ranking potential binding affinity based on complementarity of cubic quantizations of affinity regions to potential ligands.

27. An apparatus comprising a computer-readable storage medium, and program data encoded in the medium for operating on a model of a three dimensional surface, and determining concave areas on the surface of the three dimensional model including intersecting the surface with a number of planar slices, determining for at least two slices a parameter based on the intersection between the surface and the slices, and using the determinations to determine a preferred concave area on the surface.

28. A system comprising a computing system for displaying a three dimensional computer surface and for determining concave areas on the surface including intersecting the surface with a number of planar slices, determining for at least two slices a parameter based on the intersection between the surface and the slices, and using the determinations to determine a preferred concave area of the surface.